Enthalpy Change ($\Delta H)$: is the heat change at constant pressure. Usually quoted in KJ/mol.

Exothermic Reaction	ΔH = -ve	Releases heat energy from system to surroundings. Temperature of surroundings increases.	$C_5H_{12} + 8O_2 - 5CO_2 + 6H_2O$	H Reactants AH Products Reaction Progress
Endothermic Reaction	ΔH = +ve	Takes in heat energy from surroundings to system. Temperature of surroundings decreases.	$CaCO_3 \longrightarrow CaO + CO_2$	H Reactants Reaction Progress

Key Definitions

Standard Enthalpy change of Formation ($\Delta H_f \Theta$): is the enthalpy change when one mole of a substance is formed from its constituent elements under standard conditions, with all reactants and products in their standard states

$$Na_{(s)} + \frac{1}{2} Cl_{2(g)} - - - \rightarrow NaCl_{(s)}$$

 $2Na_{(s)} + Cl_{2(g)} - - - \rightarrow 2NaCl_{(s)}$ incorrect as not one mole formed as per definition.

Standard Enthalpy change of Combustion ($\Delta H_c \Theta$): is the enthalpy change when one mole of substance is completely burned/combusted in oxygen under standard conditions, with all reactants and products in their standard states

$$C_3H_{8(g)} + 5O_{2(g)} - - - \rightarrow 3CO_{2(g)} + 4H_2O_{(l)}$$

Note:

Standard enthalpy of formation of elements is 0 KJ/mol e.g. Mg, O_2 Standard enthalpy of combustion of Oxygen is 0 KJ/mol. Standard conditions (Θ) refer to Temperature: 298K, Pressure: 100kPa

Calculating Enthalpy change of a reaction

The enthalpy change of a reaction can be calculated in the following ways where applicable:

- 1) Hess's Law
- 2) Calorimetry
- 3) Mean Bond Enthalpies

Hess' Law

Hess's Law states that the enthalpy change of a reaction is independent of the route taken.







Example 1

$$\label{eq:lambda} \begin{split} \mbox{Calculate the standard enthalpy change of the combustion of Propane, given the following data:} \\ \Delta H_f[C_3H_8] = -104.7 \ \rm KJ/mol \qquad \Delta H_f[CO_2] = -393.5 \ \rm KJ/mol \qquad \Delta H_f[H_2O] = -285.8 \ \rm KJ/mol \ \Delta H_f[H_2O] =$$



 $\Delta {\rm H_r} = 104.7 + \ -2323.7 = -2,219 \ KJ/mol$

Note: The question states to calculate the enthalpy change of combustion of Propane. This does not mean we use a combustion system. The system we use depends on the enthalpy values provided. In this case we are provided with enthalpy of formation values, hence use a formation system.

Example 2



 $\Delta {\rm H_r} = -3,\!895 + \ +3,\!907 = +12 \ KJ/mol$

Note: The question states to calculate the enthalpy of formation of Methylbenzene (C_7H_8) , but we use a combustion Hess' law system as the values provided are standard enthalpy of combustion values. Also, note the combustion products in this case are Carbon dioxide and Water.

Key Notes

In certain cases, the enthalpy changes of combustion/formation will be given to you in the form of an equation i.e. you have to be able to identify whether this is ΔH_f or ΔH_c . In some cases, a reaction can represent both an enthalpy of formation of one substance, but enthalpy of combustion of another. Let's look at a few examples:

Reaction Equation	Standard Enthalpy of Formation?	Standard Enthalpy of Combustion?
1	YES- This equation represents the formation of	YES- This equation also represents the complete
$C_{(s)} + \frac{1}{2}O_{2(q)} \rightarrow CO_{2(q)}$	one mol of Carbon dioxide from its constituent	combustion of Carbon as one mole is completely
	elements.	burned/combusted.
	YES- This equation represents the formation of	YES- This equation also represents the complete
$H_{2(a)} + \frac{1}{2}O_{2(a)} \rightarrow H_2O_{(l)}$	one mol of Water from its constituent elements.	combustion of Hydrogen as one mole is
2(g) 2 2(g) 2 (o)		completely burned/combusted.
	NO- Does not represent the enthalpy of formation	YES- This equation also represents the complete
$N_{2(g)} + 2O_{2(g)} \rightarrow 2NO_{2(g)}$	of Nitrogen dioxide, as 2 moles are formed.	combustion of Nitrogen as one mole is completely
		burned/combusted.



Calorimetry

The Enthalpy change of a reaction can also be calculated experimentally via calorimetry. The general equation used to calculate the energy change is:

$$Q = m \ge c \ge \Delta T$$

Where:

Q = heat change (J)

m = mass of substance being heated or cooled (g)

 $c = specific heat capacity (Jg^{-1}K^{-1})$: states the energy required to raise the temperature of 1g of a substance by 1K.

 ΔT = temperature change (K)

In order to calculate enthalpy change, recall units are KJ/mol, we divide Q by mol. Ensure to convert Q from Joules to KJ by dividing by 1000.

$$\Delta \mathbf{H} = \frac{\mathbf{Q}}{\mathbf{n}} = \frac{KJ}{mol}$$

Calculating enthalpy of combustion

A fuel can be burned in order to heat a pre-determined mass of water to calculate the enthalpy change of combustion of the fuel.

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Example 3

4.6 of Ethanol was completely burned to raise the temperature of 100 cm³ of Water from 20°C to 28°. Calculate the enthalpy change of combustion?

First calculate the heat change:

$$Q = m \ge c \ge \Delta T$$

 $Q = 100 \ge 4.18 \ge 8$
 $Q = 3,344 J = 3.344 KJ$

In order to calculate the energy released per mole, we need to calculate the moles of ethanol:

$$=\frac{mass(g)}{Mr}=\frac{4.6}{46}=0.1$$
 moles

The enthalpy change of combustion in KJ/mol can be calculated as follows:

$$\Delta H = \frac{Q}{n} = \frac{3.344}{0.1} = -33.44 \text{KJ/mod}$$

Note, a negative sign is included in the answer, as combustion is an exothermic reaction i.e. temperature of the surrounding (water) goes up.

Discrepancies in this method include: incomplete combustion of fuel, heat loss, evaporation of fuel post weighing, non-standard conditions.

Example 4 - Calculating enthalpy change of neutralisation reactions

30cm³ of 0.6mol/dm³ HCl was added to 20cm³ of 0.5mol/dm³ of KOH. The temperature of the solution increased from 20°C to 27.2°C. Calculate the enthalpy change of the reaction:

First calculate the heat change:

$$Q = m \ge c \ge \Delta T$$

$$Q = 50 \ge 4.18 \ge 7.2$$

$$Q = 1,504.8 I = 1.5048 KI$$

In order to calculate the energy released per mole, we need to calculate the moles of HCl and KOH, to identify which is the limiting reactant.

$$moles \ of \ HCl = \frac{c \ x \ V(cm^3)}{1000} = \frac{0.6x \ 30}{1000} = 0.018 \ moles \qquad moles \ of \ KOH = \frac{c \ x \ V(cm^3)}{1000} = \frac{0.5 \ x \ 20}{1000} = 0.010 \ moles$$

Note only the limiting reactant contributes to the energy change, the excess mol do not react hence do not contribute to energy change. Therefore, the limiting reactant moles should be used. Note temperature of the solution increases, hence exothermic:

$$\Delta H = \frac{Q}{n} = \frac{1.5048}{0.01} = -150.48 KJ/mol$$

Example 5- Calculating enthalpy change of displacement reactions

5g of Zn is added to $25cm^3$ of $0.6 \text{ mol/dm}^3 \text{ CuSO}_4$ soln. The temperature of the solution increases by 5.5K. Calculate the enthalpy change of the reaction?

First calculate the heat change:

$$Q = m \ge c \ge \Delta T$$

$$Q = 25 \ge 4.18 \ge 5.5 = 574.5J = 0.575KJ$$

In order to calculate the energy released per mole, we need to calculate the moles of Zn and CuSO₄, to identify which is the limiting reactant.

moles of
$$Zn = \frac{mass(g)}{Ar} = \frac{5}{65.4} = 0.0765 \text{ moles}$$

moles of $CuSO_4 = \frac{c \times V(cm^3)}{1000} = \frac{0.6 \times 25}{1000} = 0.015 \text{ moles}$

Note only the limiting reactant contributes to the energy change, the excess mol do not react hence do not contribute to energy change. Therefore, the limiting reactant moles should be used:

$$\Delta H = \frac{Q}{n} = \frac{0.575}{0.015} = -38.3 KJ/mol$$

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Bond Enthalpies

Bond Dissociation Enthalpy: is the enthalpy change required to break one mol of a covalent bond with all species in their gaseous state. **Mean Bond Enthalpy**: average value of the bond dissociation enthalpy for a given bond taken from a range of different compounds.

 $Cl_{2(g)} - - - - \rightarrow 2 Cl_{(g)}$ $\Delta H = 242 KJ/mol$

Note: Bond enthalpy values are always positive, as energy is required to break the bond. Bond Breaking= endothermic. Bond forming= exothermic.

To calculate enthalpy change of a reaction using bond enthalpies, use the below formulae:

$$\Delta H = \sum$$
 Bonds energies of bonds broken – \sum Bonds energies of bonds formed

Example 6

Calculate the enthalpy change of combustion of Pentane using the data table provided below?



Note: Drawing a displayed formula of the reactants and products helps with visualisation of the no. of bonds present in the respective reactants and products. Highly recommend this.

